

## The curvature perturbation at second order

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# The curvature perturbation at second order

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**Abstract.** We give an explicit relation, up to second-order terms, between scalar-field fluctuations defined on spatially-flat slices and the curvature perturbation on uniform-density slices. This expression is a necessary ingredient for calculating observable quantities at second-order and beyond in multiple-field inflation. We show that traditional cosmological perturbation theory and the ‘separate universe’ approach yield equivalent expressions for superhorizon wavenumbers, and in particular that all nonlocal terms can be eliminated from the perturbation-theory expressions.

**Keywords:** inflation, cosmological perturbation theory

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## 1 Introduction

According to our current ideas, structure in the universe was seeded by quantum fluctuations which were amplified during an inflationary epoch. During inflation these fluctuations dominate the variation in energy density from place to place and therefore generate a gravitational response which can be probed by cosmological observations.

Inflationary amplification is believed to occur for any sufficiently light degree of freedom, in the sense that its mass  $m$  was substantially less than the Hubble rate  $H$  while scales of interest were being carried beyond the horizon. Models motivated by modern concepts in high-energy physics often invoke many light fields, and therefore can be tested only if we have an understanding of their effects. The literature surrounding calculations of the inflationary density perturbation is now very mature — often with agreement on subtle effects to second- or even third-order in perturbation theory — which allows these effects to be predicted in some detail. But despite this maturity it is remarkable that no completely explicit formula has been given for the uniform-density gauge curvature perturbation in an inflationary model with an arbitrary number of fields.<sup>1</sup> A formula of this type would give the next-order term in the classic result  $\zeta = -\dot{\phi}_\alpha \delta\phi^\alpha / 2M_{\text{P}}^2 H \epsilon$  which has long been known at first order. It is a key element in computing non-Gaussian signatures in the statistics of the inflationary density perturbation. Here and below,  $\epsilon \equiv -\dot{H}/H^2$  is the usual slow-roll parameter and  $\delta\phi^\alpha$  labels the species of light fields.

In this paper we supply the missing formula, valid for an arbitrary number of canonical fields and without using the slow-roll approximation. We perform the calculation using two independent methods: traditional ‘cosmological perturbation theory’, which is an expansion in the amplitude of small fluctuations around a Robertson-Walker background, and the ‘separate universe approach’, which is an expansion in the amplitude of *gradients* of the

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<sup>1</sup>Maldacena computed the second-order version of this relationship in a single-field, canonical model of inflation [1]. Some results are known to second- or even third-order for multiple-field scenarios, but typically these invoke the slow-roll approximation or do not explicitly specialize to a scalar field model. See, eg. Malik [2]. Anderson et al. gave results to third order for superhorizon scales using the slow-roll expansion [3]. A geometrical description of the large-scale, second-order gauge transformation based on curvatures in the phase-space of solutions was given in ref. [4].

perturbations. In practice (although not required in principle), separate-universe calculations often invoke a second expansion in the amplitude of the fluctuations, after which the two methods should agree for any Fourier mode much larger than the cosmological horizon. For a mode of wavenumber  $\mathbf{k}$  this requires  $k/aH \ll 1$ , making spatial gradients negligible. We verify that the two approaches give equivalent answers and clarify some issues regarding nonlocal terms which appear in the perturbation theory expressions.

Our final expressions will be used in forthcoming papers which describe numerical calculation of the two- and three-point functions in multiple-field inflation.

While the final version of this paper was being prepared, a preprint by Christopherson, Nalson & Malik appeared in which the second-order gauge transformation was given explicitly for a scalar field model [5]. We comment on the relation between our results in section 4.

**Notation.** We work in units where  $c = \hbar = 1$ . Newton’s constant is expressed in terms of the reduced Planck mass,  $M_{\text{P}}^2 = (8\pi G)^{-1}$ . Spacetime indices are labelled with Greek letters from the middle of the alphabet,  $\mu, \nu, \dots$ , and spatial indices are labelled with Latin indices from the middle of the alphabet,  $i, j, \dots$ . The different species of scalar field are labelled with Greek letters from the beginning of the alphabet,  $\alpha, \beta, \dots$ .

## 2 Cosmological gauges

The unperturbed cosmology is taken to be described by a spatially flat Robertson-Walker metric

$$ds^2 = -dt^2 + a(t)^2 d\mathbf{x}^2, \quad (2.1)$$

where  $a(t)$  is the scale factor and  $H = \dot{a}/a$  is the Hubble parameter. An overdot denotes a derivative with respect to cosmic time  $t$ .

**Choice of slicing.** In the unperturbed universe, spatial hypersurfaces of fixed time  $t$  are associated with a number of physical properties: they are slices of uniform energy density, uniform Hubble parameter, zero intrinsic Ricci curvature, and so on. Once we add perturbations these hypersurfaces continue to exist but typically no longer coincide. To compare the value of some physical quantity such as the density  $\rho$  between the perturbed and unperturbed universes we pick one set of hypersurfaces to use as a reference. This is said to be a *choice of slicing*. The perturbation in a physical quantity is defined to be the difference between its value on the same hypersurface in the perturbed and unperturbed universes.

A choice of slicing, together with a rule for determining the spatial coordinates on each slice, is called a choice of gauge. In principle we can fix the slicing and use whatever coordinate system we like to describe it, but in practice it is convenient to choose coordinates so that slices of constant  $t$  coincide with the slicing. We describe coordinates with this property as *adapted to the slicing*. Having chosen a slicing, the metric can be written in adapted coordinates using Arnowitt-Deser-Misner (ADM) quantities,

$$ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt), \quad (2.2)$$

where  $N$  is the lapse function and  $N_i$  the shift vector. The spatial metric  $h_{ij}$  is used to raise and lower spatial indices, eg.  $N_i = h_{ij}N^j$ . The curvature perturbation associated with this

slicing, denoted  $\psi$ , is defined by<sup>2</sup>

$$e^{6\psi} \equiv \det(h_{ij}/a^2). \quad (2.3)$$

A number of slicings are commonly used in the literature. The most important are:

- **Spatially flat slicing.** This has  $\det(h_{ij}/a^2) = 1$  and therefore  $\psi$  is identically zero. In the absence of gravitational waves there exist coordinates for which  $h_{ij} = a^2\delta_{ij}$ . The Ricci curvature of each spatial hypersurface is zero.

If gravitational waves are present then  $h_{ij} = a^2 e^{\gamma_{ij}}$  where  $\gamma_{ij}$  is transverse and traceless. This preserves the condition  $\det(h_{ij}/a^2) = 1$  but the Ricci curvature is no longer zero. In this context we should more properly speak of a ‘uniform Hubble slicing’.

- **Comoving slicing.** This is chosen so that there is no net energy flux measured on a fixed slice. Applied to the energy-momentum tensor in a holonomic basis adapted to the slicing this implies  $T_{0i} = 0$ . The curvature perturbation defined by this slicing is conventionally denoted  $\mathcal{R}$ .<sup>3</sup>
- **Uniform density slicing.** The density  $\rho$  is constant on a fixed slice. The curvature perturbation is conventionally written  $\zeta$ . In the absence of gravitational waves, coordinates exist in which the spatial metric can be written  $h_{ij} = a^2 e^{2\zeta} \delta_{ij}$ .

It is known that  $\mathcal{R}$  and  $\zeta$  agree on superhorizon scales up to second order, in the sense that  $(\mathcal{R} - \zeta)_{\leq 2} = \mathcal{O}(k/aH)^2$  [6], where the subscript ‘ $\leq 2$ ’ denotes terms of second order or less. We will reproduce the first-order version of this result by direct calculation in section 2.3 below. In this paper we focus on  $\zeta$  because it is known to be conserved to all orders in perturbation theory (including quantum effects) when the dynamics are adiabatic [7–12]. To our knowledge the equivalence between  $\zeta$  and  $\mathcal{R}$ , and conservation of  $\mathcal{R}$  in an adiabatic regime, have been explicitly demonstrated only to second order [13].

In the absence of isocurvature perturbations,  $\zeta$  can be used to set initial conditions for the CMB anisotropy. Therefore it represents a convenient way to express observable quantities. But inflationary calculations are often technically simplest in the spatially flat gauge, where the curvature perturbation is zero and fluctuations are measured by the scalar field perturbations  $\delta\phi^\alpha$ . If we take advantage of this simplicity then a rule is needed to connect the  $\delta\phi^\alpha$  to  $\zeta$ . As explained in section 1, our objective is to compute this rule to second order in the  $\delta\phi^\alpha$ .

This approach was used by Guth & Pi [14] and Bardeen, Steinhardt & Turner [15] in the earliest estimates of the density perturbation. These calculations exploited the technical simplicity of the flat gauge to compute the amplification of quantum effects, after which a variety of arguments were used to estimate the first-order, single-field result  $\zeta \sim -H\delta\phi/\dot{\phi}$  [14]. The relation between these methods was clarified by Lyth [16]. Later, the first-order result

<sup>2</sup>This definition is not the same as that of the review article by Malik & Wands [6]. It agrees with the quantity used at the nonlinear level by Maldacena [1]. The definition (2.3) was used to prove conservation of  $\psi = \zeta$  in the uniform density gauge at a classical level by Shellard & Rigopoulos [7], Lyth, Malik & Sasaki [8] and Weinberg [9, 10]. More recently the proof has been strengthened to an operator statement in quantum mechanics by Assassi, Baumann & Green [11].

<sup>3</sup>There are differing sign conventions for  $\mathcal{R}$ . Our definition gives  $\zeta = \mathcal{R} + \mathcal{O}(k/aH)^2$  on superhorizon scales, but other definitions reverse this to  $\zeta = -\mathcal{R} + \mathcal{O}(k/aH)^2$ .

was extended to multiple-field scenarios by Salopek & Bond [17], who used it to generate numerical results. Formulae for more complex models were given by Sasaki & Stewart using the ‘separate universe approach’ [18–20]. More recently, Maldacena computed the relationship between  $\zeta$  and  $\delta\phi$  in a single-field model and discussed its application to higher  $n$ -point functions [1].

## 2.1 Changing slicing

To connect quantities defined by different slicings, such as  $\zeta$  and  $\delta\phi^\alpha$ , we must change the gauge. In the literature this is sometimes described as a coordinate transformation. If not interpreted correctly this description is confusing because under a coordinate transformation any tensor transforms covariantly, and we shall see that this is not the same as the transformation law under a change of gauge. The difference arises because to change gauge we first change the slicing and *then* change the coordinates to adapt to it.

Begin with some initial slicing and adapted coordinates  $x^\mu$ . Suppose we wish to switch to a different set of slices which are slightly displaced. At any point  $p$  the displacement to the matching point  $p'$  on the new surface is written

$$x^\mu(p) \rightarrow x^\mu(p') = e^{\mathcal{L}_\xi} x^\mu(p). \quad (2.4)$$

The Lie derivative  $\mathcal{L}_\xi$  is understood to act on the coordinates  $x^\mu(p)$  as if they were the components of a contravariant vector field. This abuse of notation is unfortunate but conventional. The vector  $\xi^\mu$  associated with the Lie derivative is called the gauge parameter. Given two slicings our task will usually be to solve for an appropriate gauge parameter.

Now introduce a second set of coordinates  $x^{\bar{\mu}}$  adapted to the new slicing, with the time coordinate adjusted so that the numerical value of time agrees on both slices. We distinguish indices associated with these new coordinates using a bar. By a ‘gauge transformation’, we mean a map from tensors at  $p$  expressed in the holonomic basis  $\{dx^\mu, \partial/\partial x^\mu\}$  to tensors at  $p'$  expressed in the holonomic basis  $\{dx^{\bar{\mu}}, \partial/\partial x^{\bar{\mu}}\}$ . This is both a change of evaluation point and a change of basis.

To define the map, consider a generic tensor  $\mathbf{T}$  at  $p$ . In the original basis its components are

$$\mathbf{T}|_p = T_{\mu\dots}{}^{\nu\dots}(p) dx^\mu|_p \otimes \dots \otimes \frac{\partial}{\partial x^\nu}\bigg|_p \otimes \dots. \quad (2.5)$$

The gauge transformation yields a transformed tensor  $\mathbf{T}'$  at  $p'$ ,

$$\mathbf{T}'|_{p'} = T_{\bar{\mu}\dots}{}^{\bar{\nu}\dots}(p') dx^{\bar{\mu}}|_{p'} \otimes \dots \otimes \frac{\partial}{\partial x^{\bar{\nu}}}\bigg|_{p'} \otimes \dots. \quad (2.6)$$

The map between the components, expressed in these different bases, is

$$T_{\mu\dots}{}^{\nu\dots}(p) \rightarrow T_{\bar{\mu}\dots}{}^{\bar{\nu}\dots}(p') = e^{\mathcal{L}_\xi} T_{\mu\dots}{}^{\nu\dots}(p) \quad (2.7)$$

where one should identify matching index labels  $\mu \rightarrow \bar{\mu}$  (and so on), and on the right-hand

side the Lie derivative is understood to mean its action on the components of  $\mathbf{T}$  in the original basis.<sup>4</sup>

In the context of perturbation theory, the displacement between hypersurfaces is small and therefore so is the gauge parameter  $\xi^\mu$ . In this paper we are interested in computing the relationship between quantities defined on different slicings up to second order in amplitude. Hence, we must work to the same order in powers of  $\xi^\mu$ . We break  $\xi^\mu$  into temporal and spatial gauge parameters  $\xi^0$  and  $\xi^j$ , corresponding to the time and space components of  $\xi^\mu$ .

**Transformation of field fluctuations.** Using eq. (2.7) we can compute how each quantity of interest transforms between slicings. A field fluctuation  $\delta\phi^\alpha$  transforms according to the rule

$$\delta\phi^\alpha(t') = \delta\phi^\alpha(t) + \xi^0 \dot{\phi}^\alpha + \xi^0 \frac{\partial \delta\phi^\alpha(t)}{\partial t} + \xi^j \partial_j \delta\phi^\alpha(t) + \frac{(\xi^0)^2}{2} \ddot{\phi}^\alpha + \frac{\dot{\phi}^\alpha}{4} \frac{\partial (\xi^0)^2}{\partial t}. \quad (2.11)$$

On the right-hand side,  $\dot{\phi}^\alpha$ ,  $\ddot{\phi}^\alpha$  (and so on) represent derivatives of the background field with respect to time. Because we adjusted the time coordinates of the slices to agree it is not necessary to specify whether the derivatives are with respect to  $t$  or  $t'$ . The symbols  $\delta\phi^\alpha(t)$  and  $\delta\phi^\alpha(t')$  denote, respectively, field fluctuations defined on the first slicing of constant  $t$ , and the second slicing of constant  $t'$ .

The time derivative of a field fluctuation transforms according to

$$\begin{aligned} \frac{\partial \delta\phi^\alpha(t')}{\partial t'} &= \frac{\partial \delta\phi^\alpha(t)}{\partial t} + \xi^0 \frac{\partial^2 \delta\phi^\alpha(t)}{\partial t^2} + \xi^j \partial_j \frac{\partial \delta\phi^\alpha(t)}{\partial t} + \frac{\partial \xi^0}{\partial t} \frac{\partial \delta\phi^\alpha(t)}{\partial t} + \frac{\partial \xi^j}{\partial t} \partial_j \delta\phi^\alpha(t) \\ &\quad + \ddot{\phi}^\alpha \xi^0 + \frac{1}{2} \ddot{\phi}^\alpha (\xi^0)^2 + \dot{\phi}^\alpha \frac{\partial \xi^0}{\partial t} + \frac{3}{4} \ddot{\phi}^\alpha \frac{\partial (\xi^0)^2}{\partial t} + \frac{\ddot{\phi}^\alpha}{2} \xi^j \partial_j \xi^0 \\ &\quad + \frac{\dot{\phi}^\alpha}{4} \frac{\partial^2 (\xi^0)^2}{\partial t^2} + \frac{\dot{\phi}^\alpha}{2} \frac{\partial}{\partial t} (\xi^j \partial_j \xi^0). \end{aligned} \quad (2.12)$$

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<sup>4</sup>Note that this map must be phrased carefully. In the literature of ‘active’ gauge transformations, which is the point of view being adopted here, one sometimes finds the statement

$$\mathbf{T} \rightarrow \mathbf{T}' = e^{\mathcal{L}_\xi} \mathbf{T}. \quad (2.8)$$

To see that this can be made to agree with our eq. (2.7) requires an extra assumption. The action of the Lie derivative on the tensor  $\mathbf{T}$  defined in (2.5) yields another tensor at  $p$ ,

$$\mathcal{L}_\xi \mathbf{T} = \mathcal{L}_\xi \left( T_{\mu\dots}{}^{\nu\dots}(p) dx^\mu|_p \otimes \dots \otimes \frac{\partial}{\partial x^\nu} \Big|_p \otimes \dots \right) = [\mathcal{L}_\xi T_{\mu\dots}{}^{\nu\dots}]_p dx^\mu|_p \otimes \dots \otimes \frac{\partial}{\partial x^\nu} \Big|_p \otimes \dots. \quad (2.9)$$

The notation  $\mathcal{L}_\xi T_{\mu\dots}{}^{\nu\dots}$  denotes the action of the Lie derivative in a coordinate basis; for example, for a one-form or covariant vector,  $\mathcal{L}_\xi \omega_a = \xi^b \partial_b \omega_a + \omega_b \partial_a \xi^b$ . To obtain a tensor evaluated at  $p'$  from (2.9) requires a separate rule, which is the extra assumption described above.

One option is to use the push-forward or Jacobian map, which would undo part of the action of the Lie derivative. This is defined using the Jacobian map to pull back the basis at  $p'$  to  $p$ , so after doing so the components would be related only by a change of evaluation point,

$$\mathcal{L}_\xi \mathbf{T} \xrightarrow{\text{Jacobian map}} T_{\mu\dots}{}^{\nu\dots}(p') dx^\mu|_{p'} \otimes \dots \otimes \frac{\partial}{\partial x^\nu} \Big|_{p'} \otimes \dots. \quad (2.10)$$

This reproduces the starting point for the gauge transformation, described above eq. (2.5). Therefore, after changing basis to  $(dx^\mu)_{p'}$ ,  $(\partial/\partial x^\mu)_{p'}$  and exponentiating the Lie derivative operator, one will again arrive at eq. (2.7).



**Transformation of metric components.** We also require transformation rules for the metric components  $N$ ,  $N^i$  and  $h_{ij}$ . Bearing in mind that we intend to compute  $\zeta$  in terms of the flat-gauge perturbations  $\delta\phi^\alpha$  we simplify these expressions by assuming that the initial slicing corresponds to the flat gauge where  $h_{ij} = a^2\delta_{ij}$ . We do not yet impose any restriction on the final slicing.

Instead of working with the lapse directly it is more convenient to work in terms of its perturbation  $\alpha$ , defined by  $N \equiv 1 + \alpha$ . The transformation rule for  $\alpha$  is<sup>5</sup>

$$\begin{aligned} \alpha' = \alpha &+ \frac{\partial\xi^0}{\partial t} + \frac{1}{4}\frac{\partial^2(\xi^0)^2}{\partial t^2} + \frac{1}{2}\frac{\partial}{\partial t}\left(\xi^j\partial_j\xi^0\right) + \frac{\partial(\alpha\xi^0)}{\partial t} + \xi^j\partial_j\alpha - N^m\partial_m\xi^0 \\ &+ \frac{1}{2a^2}\partial_i\xi^0\partial_i\xi^0 - \partial_i\xi^0\frac{\partial\xi^i}{\partial t}. \end{aligned} \quad (2.13)$$

Likewise, the transformation rule for the shift vector is

$$\begin{aligned} N_{j'} = N_j &- \partial_j\xi^0 - \frac{1}{4}\partial_j\frac{\partial(\xi^0)^2}{\partial t} - \frac{1}{2}\partial_j(\xi^m\partial_m\xi^0) - \frac{\partial\xi^0}{\partial t}\partial_j\xi^0 - 2\alpha\partial_j\xi^0 + N_j\frac{\partial\xi^0}{\partial t} \\ &+ N_m\partial_j\xi^m + \xi^0\frac{\partial N_j}{\partial t} + \xi^m\partial_m N_j \\ &+ a^2\left(\delta_{jm}(1+2H\xi^0)\frac{\partial\xi^m}{\partial t} + \delta_{mn}\frac{\partial\xi^m}{\partial t}\partial_j\xi^n + \frac{\delta_{jm}}{2}\frac{\partial}{\partial t}\left[\xi^0\frac{\partial\xi^m}{\partial t} + \xi^n\partial_n\xi^m\right]\right). \end{aligned} \quad (2.14)$$

Finally, the spatial metric transforms according to

$$\begin{aligned} h_{i'j'} = a^2(1+2H\xi^0)\delta_{ij} &- \partial_i\xi^0\partial_j\xi^0 + N_i\partial_j\xi^0 + N_j\partial_i\xi^0 \\ &+ a^2\left((1+2H\xi^0)(\delta_{im}\partial_j + \delta_{jm}\partial_i)\xi^m + \left[\frac{\delta_{im}}{2}\partial_j + \frac{\delta_{jm}}{2}\partial_i\right]\left[\xi^0\frac{\partial\xi^m}{\partial t} + \xi^n\partial_n\xi^m\right] \right. \\ &\left. + \delta_{mn}\partial_i\xi^m\partial_j\xi^n + \delta_{ij}(2H + \dot{H})(\xi^0)^2 + \frac{\delta_{ij}}{2}H\frac{\partial(\xi^0)^2}{\partial t}\right). \end{aligned} \quad (2.15)$$

From (2.3) and (2.15) we can compute the curvature perturbation in the new slicing. It is

$$\begin{aligned} \psi' = H\xi^0 &+ \frac{1}{3}\partial_j\xi^j - \frac{1}{6a^2}\partial_j\xi^0\partial_j\xi^0 + \frac{1}{3}N^m\partial_m\xi^0 + \frac{1}{6}\partial_j\xi^0\frac{\partial\xi^j}{\partial t} + \frac{1}{6}\xi^0\frac{\partial(\partial_j\xi^j)}{\partial t} \\ &+ \frac{1}{6}\xi^m\partial_m\partial_j\xi^j + \frac{H}{4}\frac{\partial(\xi^0)^2}{\partial t} + \frac{\dot{H}}{2}(\xi^0)^2. \end{aligned} \quad (2.16)$$

The definition  $\psi \sim \det h/a^2$  implies that the curvature perturbation measures modulation in proper volume from place to place on a fixed slice. Eq. (2.16) exhibits the expected invariance under volume-preserving transformations of the spatial coordinates which do not change the slicing. These are generated by gauge transformations with  $\xi^0 = 0$  and divergenceless  $\xi^j$ , *viz.*  $\partial_j\xi^j = 0$ . They include the spatial rotations.

Gauge transformations with  $\xi^0 \neq 0$  change the slicing. For such transformations there is a small second-order volume modulation even if  $\xi^j$  is divergenceless, provided it is time-dependent and  $\xi^0$  is spatially dependent. This arises from the second-to-last term in the first line of (2.16). If  $\xi^j$  is time-independent there is no modulation, and no contribution to the curvature perturbation. Eq. (2.14) shows that a time-independent transformation of this kind

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<sup>5</sup>Contraction of repeated indices in the lowered position implies summation with the Euclidean metric  $\delta_{ij}$ .

negligibly perturbs the shift-vector  $N^j$  when all  $\mathbf{k}$ -modes are associated with superhorizon scales for which  $k/aH \ll 1$ .<sup>6</sup>

**Restriction to diagonal metric.** Normally only  $\xi^0$  is needed to select the slicing of interest, leaving  $\xi^j$  undetermined. As described above, this ambiguity is irrelevant if  $\xi^j$  becomes time-independent and volume-preserving when all modes are superhorizon. More generally we could choose  $\xi^j$  to bring  $h_{ij}$  to a diagonal form. This requires the first-order perturbation to satisfy  $\partial_i \xi_1^i = 0$ , which forces  $\xi_1^i$  to be spatially homogeneous (but perhaps time-dependent) and therefore volume-preserving. At second order the diagonal constraint is more complex, but entails

$$\partial_j \xi_2^j = \frac{1}{2a^2} \partial_j \xi^0 \partial_j \xi^0 - N^j \partial_j \xi^0 - \frac{1}{2} \partial_j \xi^0 \frac{\partial \xi^j}{\partial t}. \quad (2.17)$$

When  $\xi^j$  is chosen to satisfy (2.17) it can be checked that  $\psi'$  becomes independent of its precise value. We find

$$\psi'^{\text{diagonal}} \equiv H \xi^0 + \frac{H}{4} \frac{\partial (\xi^0)^2}{\partial t} + \frac{\dot{H}}{2} (\xi^0)^2. \quad (2.18)$$

The right-hand side of (2.17) decays when all wavenumbers are associated with superhorizon scales. Therefore, on these scales, any rigid volume-preserving spatial gauge transformation leaves  $h_{ij}$  diagonal and allows  $\psi'$  to be computed using the simplified expression (2.18). Conversely, because different possibilities for  $\xi^j$  change  $\psi'$  when  $k/aH \gtrsim 1$  there is no unique value of the curvature perturbation associated with subhorizon scales. In practice this is harmless because on these scales  $\psi'$  has no clear significance.

## 2.2 Spatially flat slicing

Now we apply this formalism to translate between the spatially flat slicing and the uniform-density slicing. In the language of section 2.1, slices of constant  $t$  correspond to the flat gauge and slices of constant  $t'$  correspond to the uniform density gauge. The transformed curvature perturbation  $\psi'$  will be  $\zeta$ .

We begin from coordinates in which the flat-gauge spatial metric is diagonal, *viz.*  $h_{ij} = a^2 \delta_{ij}$ . We choose  $\xi^0$  to select an appropriate final slicing and assume that the spatial gauge transformation is chosen to satisfy (2.17).

**Lapse and shift.** Before embarking on the calculation, we use this section to collect formulae for the lapse and shift in the spatially flat gauge. Eq. (2.16) shows that these are not directly required to compute  $\zeta$  — this expression does not contain  $\alpha$ , and its  $N^j$  dependence drops out when all wavenumbers are associated with superhorizon scales. However, they are required indirectly because the density perturbation which will be used to determine  $\xi^0$  depends on the metric. Moreover, the lapse and shift are elements in an important constraint equation — the Hamiltonian constraint — which we will use later to simplify our results.

We work perturbatively in the scalar field fluctuation  $\delta\phi^\alpha$ . We break the shift vector  $N_j$  into irrotational and solenoidal components  $\vartheta$  and  $\beta_j$ ,

$$N_j \equiv \partial_j \vartheta + \beta_j \quad (2.19)$$

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<sup>6</sup>Our interest lies in using the second-order gauge transformation to compute three- and higher  $n$ -point correlation functions of  $\zeta$ . For this purpose we need an expression such as (2.14) only in the case where each  $\xi^0(\mathbf{k})$  mode individually satisfies  $k/aH \ll 1$ , making decay obvious term-by-term. A more general theorem was proved by Weinberg [9, 10].

where  $\partial_j \beta_j = 0$ . Then  $\vartheta$ ,  $\beta_j$  and the lapse perturbation  $\alpha$  can be expanded in powers of  $\delta\phi^\alpha$ , giving

$$\alpha \equiv \sum_{n=1}^{\infty} \alpha_n, \quad \vartheta \equiv \sum_{n=1}^{\infty} \vartheta_n \quad \text{and} \quad \beta_j \equiv \sum_{n=1}^{\infty} \beta_{n|j} \quad (2.20)$$

where the term  $\alpha_n$  contains exactly  $n$  factors of  $\delta\phi$ , and likewise for  $\vartheta_n$  and  $\beta_{n|j}$ .

We neglect tensor perturbations, which correspond to gravitational waves. These could be kept but because they are represented by transverse traceless tensors  $\gamma_{ij}$  and are uncorrelated with the field fluctuations at tree-level they do not enter connected tree-level autocorrelation functions of  $\zeta$  lower than the trispectrum. With these choices the lapse perturbations satisfy [1, 21, 22]

$$\alpha_1 = \frac{\dot{\phi}_\alpha \delta\phi^\alpha}{2M_{\text{P}}^2 H} \quad (2.21a)$$

$$\alpha_2 = \frac{\alpha_1^2}{2} + \frac{\partial^{-2}}{2HM_{\text{P}}^2} \left( \partial_j \delta\phi^\alpha \partial_j \delta\phi_\alpha + \delta\phi^\alpha \partial^2 \delta\phi_\alpha + \frac{1}{a^2} \partial^2 \alpha_1 \partial^2 \vartheta_1 - \frac{1}{a^2} \partial_i \partial_j \alpha_1 \partial_i \partial_j \vartheta_1 \right). \quad (2.21b)$$

This expression for  $\alpha_2$  already signals a potential difficulty because it involves the nonlocal inverse Laplacian  $\partial^{-2}$ , defined as multiplication by  $-1/k^2$  in Fourier space. Terms of this nature cannot arise in the separate universe approach because it corresponds to an expansion in purely positive powers of  $k$ . To demonstrate that a perturbation-theory expression involving such terms is compatible with a separate-universe calculation we must show carefully how all nonlocal pieces disappear from the result. We will do this explicitly in section 2.3.

The first-order component of the scalar shift satisfies [1, 21]

$$-\frac{4H}{a^2} M_{\text{P}}^2 \partial^2 \vartheta_1 = 2V_\alpha \delta\phi^\alpha + 2\dot{\phi}^\alpha \delta\dot{\phi}_\alpha + 2\alpha_1 (6H^2 M_{\text{P}}^2 - \dot{\phi}^2), \quad (2.22a)$$

where  $\dot{\phi}^2 \equiv \dot{\phi}^\alpha \dot{\phi}_\alpha$  and  $V_\alpha \equiv \partial_\alpha V$  (and likewise for higher derivatives). At second order we have [22]

$$\begin{aligned} -\frac{4H}{a^2} M_{\text{P}}^2 \partial^2 \vartheta_2 = & \frac{1}{a^2} \partial_j \delta\phi^\alpha \partial_j \delta\phi_\alpha + V_{\alpha\beta} \delta\phi^\alpha \delta\phi^\beta + \delta\phi^\alpha \delta\dot{\phi}_\alpha - \frac{2}{a^2} \dot{\phi}^\alpha \partial_j \vartheta_1 \partial_j \delta\phi_\alpha \\ & - \frac{M_{\text{P}}^2}{a^4} \partial^2 \vartheta_1 \partial^2 \vartheta_1 + \frac{M_{\text{P}}^2}{a^4} \partial_i \partial_j \vartheta_1 \partial_i \partial_j \vartheta_1 + 2H^2 M_{\text{P}}^2 (2\alpha_2 - 3\alpha_1^2) (\epsilon - 3) \\ & - 2\alpha_1 \left( \frac{4H}{a^2} M_{\text{P}}^2 \partial^2 \vartheta_1 + 2\dot{\phi}^\alpha \delta\dot{\phi}_\alpha \right). \end{aligned} \quad (2.22b)$$

At linear order  $\beta_{1|j} = 0$ . The second-order component  $\beta_{2|j}$  can appear in scalar quantities only at third order or above because it is divergencelike, and therefore is not needed.

**Hamiltonian constraint.** Eqs. (2.22a)–(2.22b) are the first- and second-order parts of the ‘Hamiltonian constraint’, so called because in Einstein gravity it is enforced by the lapse  $N$  acting as its Lagrange multiplier. Because the lapse is associated with time reparametrization invariance the Hamiltonian constraint plays a role analogous to the Hamiltonian in conventional theory.

We are primarily interested in the case where all  $\mathbf{k}$ -modes are associated with super-horizon scales. In this limit,  $\partial^2 \vartheta_n / a^2$  decays [9, 10, 23] and the Hamiltonian constraint becomes

$$V_\alpha \delta\phi^\alpha + \frac{1}{2} V_{\alpha\beta} \delta\phi^\alpha \delta\phi^\beta + \dot{\phi}^\alpha \delta\dot{\phi}_\alpha + \frac{1}{2} \delta\dot{\phi}^\alpha \delta\dot{\phi}_\alpha + H^2 M_{\text{P}}^2 (2\alpha_1 + 2\alpha_2 - 3\alpha_1^2) (3 - \epsilon) - 2\alpha_1 \dot{\phi}^\alpha \delta\dot{\phi}_\alpha = 0. \quad (2.23)$$

### 2.3 The uniform-density curvature perturbation

In this section we compute the gauge transformation parameter  $\xi^0$ . To simplify the calculation we take  $\xi^j = 0$  from the outset. On superhorizon scales this will satisfy (2.17), giving a diagonal spatial metric and trivial lapse. In section 3 we will see that this statement (promoted to all orders in perturbation theory) is the basis of the separate universe approach.

**Density perturbation.** Each slicing defines a field of normal vectors  $n^\mu$  which are orthogonal to the slices. We normalize so that  $n^\mu n_\mu = -1$ . The density measured by an observer on a fixed spatial slice is  $\rho = T_{\mu\nu} n^\mu n^\nu$ , where  $T_{\mu\nu}$  is the energy-momentum tensor. In a holonomic basis of coordinates adapted to the slicing, this gives

$$\rho = -\frac{T^{00}}{g^{00}}. \quad (2.24)$$

Therefore, up to second order, the perturbation in the density will be

$$\delta\rho = \delta T^{00} + \rho\delta g^{00} + (\delta T^{00} + \rho\delta g^{00})\delta g^{00}. \quad (2.25)$$

Eqs. (2.24) and (2.25) apply for any slicing. Our interest lies in the uniform-density slicing, for which the density perturbation  $\delta\rho(t')$  on slices of constant  $t'$  is identically zero. Using the gauge-transformation formulae collected in section 2.1 it is possible to express  $\delta\rho(t')$  in terms of quantities defined on the original flat slices of constant  $t$ . That gives

$$\delta\rho(t') = \delta\rho(t) + \dot{\rho}\xi^0 + \delta\dot{\rho}\xi^0 + \frac{\dot{\rho}}{2}\xi^0\xi^0 + \frac{\ddot{\rho}}{2}(\xi^0)^2 - 2\left(\delta T^{0i}(t) + \rho\delta g^{0i}(t)\right)\partial_i\xi^0 + \partial_i\xi^0\partial_i\xi^0\left(T^{ij} + \rho g^{ij}\right). \quad (2.26)$$

The combination  $T^{ij} + \rho g^{ij}$  in the final bracket depends only on background quantities. Setting the left-hand side equal to zero, eq. (2.26) represents an equation for the gauge parameter  $\xi^0$  which can be solved to find the transformation between flat and uniform-density slices.

**Curvature perturbation.** The solution is

$$\begin{aligned} \xi^0 = & -\frac{\delta\rho}{\dot{\rho}} + \frac{\delta\dot{\rho}}{\dot{\rho}}\frac{\delta\rho}{\dot{\rho}} - \frac{1}{2}\frac{\delta\rho}{\dot{\rho}}\frac{\partial}{\partial t}\frac{\delta\rho}{\dot{\rho}} - \frac{1}{2}\frac{\ddot{\rho}}{\dot{\rho}}\left(\frac{\delta\rho}{\dot{\rho}}\right)^2 + \frac{2}{\dot{\rho}}(\delta T^{0i} + \rho\delta g^{0i})\frac{\partial_i\delta\rho}{\dot{\rho}} \\ & - \frac{1}{\dot{\rho}}\frac{\partial_i\delta\rho}{\dot{\rho}}\frac{\partial_j\delta\rho}{\dot{\rho}}\left(T^{ij} + \rho g^{ij}\right) \end{aligned} \quad (2.27)$$

In this expression, all perturbative quantities on the right-hand side are evaluated on spatially flat slices. After substitution in (2.16) with  $\xi^j = 0$ , we find

$$\begin{aligned} \zeta = & -H\frac{\delta\rho}{\dot{\rho}} + H\frac{\delta\dot{\rho}}{\dot{\rho}}\frac{\delta\rho}{\dot{\rho}} - \frac{H}{2}\frac{\delta\rho}{\dot{\rho}}\frac{\partial}{\partial t}\frac{\delta\rho}{\dot{\rho}} - \frac{H}{2}\frac{\ddot{\rho}}{\dot{\rho}}\left(\frac{\delta\rho}{\dot{\rho}}\right)^2 + \frac{2H}{\dot{\rho}}(\delta T^{0i} + \rho\delta g^{0i})\frac{\partial_i\delta\rho}{\dot{\rho}} \\ & - \frac{H}{\dot{\rho}}\frac{\partial_i\delta\rho}{\dot{\rho}}\frac{\partial_j\delta\rho}{\dot{\rho}}\left(T^{ij} + \rho g^{ij}\right) - \frac{1}{6a^2}\frac{\partial_i\delta\rho}{\dot{\rho}}\frac{\partial_i\delta\rho}{\dot{\rho}} - \frac{1}{3\dot{\rho}}\partial_i\vartheta_1\partial_i\delta\rho + \frac{H}{4}\left(\frac{\partial}{\partial t}\frac{\delta\rho}{\dot{\rho}}\right)^2 + \frac{\dot{H}}{2}\frac{(\delta\rho)^2}{\dot{\rho}}. \end{aligned} \quad (2.28)$$

Eq. (2.28) is one of our central results. It gives the curvature perturbation on uniform-density slices in terms of the flat-gauge density perturbation, the  $0i$  components of the flat-gauge energy-momentum tensor and metric, and the scalar part of the flat-gauge shift vector encoded in  $\vartheta_1$ . It applies for any matter content.

For applications to inflation the matter theory is given by an arbitrary number of scalar fields interacting via a potential  $V$ . The energy-momentum tensor is

$$T_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - \frac{1}{2}g_{\mu\nu}\partial^\lambda\phi\partial_\lambda\phi - g_{\mu\nu}V. \quad (2.29)$$

It gives a background density  $\rho = \dot{\phi}^2/2 + V$ . The density perturbation on flat slices is

$$\begin{aligned} \delta\rho = & -\alpha_1\dot{\phi}^2 + \dot{\phi}^\alpha\delta\dot{\phi}_\alpha + V_\alpha\delta\phi^\alpha - \dot{\phi}^\alpha\partial_i\partial_1\partial_i\delta\phi_\alpha + \frac{1}{2}\delta\dot{\phi}^\alpha\delta\dot{\phi}_\alpha - 2\alpha_1\dot{\phi}^\alpha\delta\dot{\phi}_\alpha \\ & + \frac{\dot{\phi}^2}{2}(3\alpha_1^2 - 2\alpha_2) + \frac{1}{2}V_{\alpha\beta}\delta\phi^\alpha\delta\phi^\beta + \frac{1}{2a^2}\partial_i\delta\phi^\alpha\partial_i\delta\phi_\alpha, \end{aligned} \quad (2.30)$$

and the  $0i$  component is

$$\delta T^{0i} = \frac{1}{a^2}\dot{\phi}^\alpha\partial_i\delta\phi_\alpha. \quad (2.31)$$

**Explicit expressions.** We can now give explicit expressions for the first- and second-order components of  $\zeta$ . We define these to satisfy  $\zeta = \zeta_1 + \zeta_2 + \dots$ , and as above  $\zeta_n$  contains terms with exactly  $n$  powers of the field perturbations. Dropping terms which decay when all wavenumbers correspond to superhorizon scales, we find

$$\zeta_1 = \frac{1}{6M_{\text{P}}^2 H^2 \epsilon} \left( \dot{\phi}^\alpha\delta\dot{\phi}_\alpha + V_\alpha\delta\phi^\alpha - 2M_{\text{P}}^2 H^2 \epsilon \alpha_1 \right) \quad (2.32a)$$

$$\begin{aligned} \zeta_2 = & \frac{1}{6M_{\text{P}}^2 H^2 \epsilon} \left( \frac{1}{2}\delta\dot{\phi}^\alpha\delta\dot{\phi}_\alpha + \frac{1}{2}V_{\alpha\beta}\delta\phi^\alpha\delta\phi^\beta - 2\alpha_1\dot{\phi}^\alpha\delta\dot{\phi}_\alpha + H^2 M_{\text{P}}^2 \epsilon (3\alpha_1^2 - 2\alpha_2) \right. \\ & + H^2 \zeta_1 \left[ \epsilon \left( \frac{3+\epsilon}{H} \dot{\phi}^\alpha - \frac{V_\alpha}{H^2} \right) \delta\phi^\alpha - \frac{6+\epsilon}{H^2} \dot{\phi}^\alpha\delta\dot{\phi}_\alpha \right] \\ & \left. + 3H^2 \zeta_1^2 \left[ 6M_{\text{P}}^2 \epsilon + \frac{V_\alpha \dot{\phi}^\alpha}{H^3} \right] \right). \end{aligned} \quad (2.32b)$$

These expressions are exact, except for the neglect of decaying terms. In deriving them we have made no use of the slow-roll approximation.

Eq. (2.32b) shows that, when derived using this method, the second-order curvature perturbation contains  $\alpha_2$  and therefore apparently depends on the nonlocal combination which appears in (2.21b). If true this would be perplexing. The explicit single-field expression given by Maldacena contains no such terms [1]. The resolution is that, in Maldacena's calculation, the second-order lapse was removed entirely by the Hamiltonian constraint (2.23).

The existence of constraints means that eqs. (2.32a)–(2.32b) can be written in a number of superficially different ways. One reason for doing so is that, because these rewritten formulations contain different terms, their numerical properties can differ even though they are mathematically equivalent. If we choose to exploit this freedom, however, we must remember that the Hamiltonian constraint mixes terms of different orders in the field fluctuations  $\delta\phi^\alpha$ . Therefore, in quantities which depend on both  $\zeta_1$  and  $\zeta_2$ , we must use expressions which have been simplified in the same way. Failure to do so will lead to a mismatch. In particular this applies when computing the three-point function  $\langle \zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2)\zeta(\mathbf{k}_3) \rangle$  from  $n$ -point functions of the field fluctuations.

One option is to remove  $\alpha_2$  entirely. This will leave a purely local expression comparable to the one obtained by Maldacena. This choice gives

$$\zeta_1^{\text{local}} = \frac{1}{2H^2 M_{\text{P}}^2 \epsilon (3 - \epsilon)} \left( \dot{\phi}^\alpha \delta \dot{\phi}_\alpha + V_\alpha \delta \phi^\alpha \right) \quad (2.33a)$$

$$\begin{aligned} \zeta_2^{\text{local}} = \frac{1}{2H^2 M_{\text{P}}^2 \epsilon (3 - \epsilon)} & \left( \left[ \frac{1}{2} V_{\alpha\beta} + \frac{\dot{\phi}_\alpha \dot{\phi}_\beta}{M_{\text{P}}^2} \left( \frac{9}{2\epsilon} - \frac{9}{2} + \epsilon + \frac{3 - \epsilon}{4\epsilon^2} \frac{V_\gamma \dot{\phi}^\gamma}{H^3 M_{\text{P}}^2} \right) \right] \delta \phi^\alpha \delta \phi^\beta \right. \\ & \left. + \frac{\dot{\phi}_\alpha \dot{\phi}_\beta}{H M_{\text{P}}^2} \left( \frac{3}{\epsilon} - 2 \right) \delta \phi^\alpha \delta \dot{\phi}^\beta + \frac{1}{2} \delta \dot{\phi}^\alpha \delta \dot{\phi}_\alpha \right). \end{aligned} \quad (2.33b)$$

Different forms for  $\zeta_2$  can be obtained by further use of the first-order Hamiltonian constraint. For example, the cross-term  $\delta \phi^\alpha \delta \dot{\phi}^\beta$  could be eliminated entirely at the expense of a more complex coefficient for the  $\delta \phi^\alpha \delta \phi^\beta$  term.

If we are prepared to tolerate residual nonlocal terms, we could alternatively use the Hamiltonian constraint to simplify  $\zeta_1$  and  $\zeta_2$  as much as possible. One choice is

$$\zeta_1^{\text{simple}} = - \frac{\dot{\phi}^\alpha \delta \phi_\alpha}{2H M_{\text{P}}^2 \epsilon} \quad (2.34a)$$

$$\begin{aligned} \zeta_2^{\text{simple}} = \frac{1}{6H^2 M_{\text{P}}^2 \epsilon} & \left( \frac{\dot{\phi}_\alpha \dot{\phi}_\beta}{M_{\text{P}}^2} \left[ -\frac{3}{2} + \frac{9}{2\epsilon} + \frac{3}{4\epsilon^2} \frac{V_\gamma \dot{\phi}^\gamma}{M_{\text{P}}^2 H^3} \right] \delta \phi^\alpha \delta \phi^\beta + \frac{3}{H\epsilon} \frac{\dot{\phi}_\alpha \dot{\phi}_\beta}{M_{\text{P}}^2} \delta \phi^\alpha \delta \dot{\phi}^\beta \right. \\ & \left. - 3H \partial^{-2} \left[ \partial_j \delta \dot{\phi}^\alpha \partial_j \delta \phi_\alpha + \delta \dot{\phi}^\alpha \partial^2 \delta \phi_\alpha \right] \right). \end{aligned} \quad (2.34b)$$

As above the  $\delta \phi^\alpha \delta \dot{\phi}^\beta$  terms can be removed, if desired, using the first-order constraint. This form of  $\zeta_1$  is especially simple, being the multiple-field generalization of the estimate  $\zeta \sim H \delta \phi / \dot{\phi}$  obtained in early calculations [14–16]. It coincides with the first-order expression obtained by direct calculation of the comoving-gauge curvature perturbation  $\mathcal{R}$ , and therefore reproduces the first-order relation  $\zeta_1 = \mathcal{R}_1$  on superhorizon scales which was discussed in section 2. Because it requires the constraint equations this relationship is a consequence of Einstein gravity and need not hold more generally.

Eqs. (2.33a)–(2.33b) and (2.34a)–(2.34b) are exactly equivalent. Neither involves any form of approximation except that because we have neglected terms which decay when all wavenumbers are associated with superhorizon scales they are valid only in this limit. Which we use is a matter of our own convenience. The only thing we cannot do is mix (for example) the simple first-order expression  $\zeta_1^{\text{simple}}$  with the local second-order result  $\zeta_2^{\text{local}}$ , or vice-versa.

Which set is most convenient will depend on the problem at hand. Eq. (2.34b) shows that it is possible to compute the curvature perturbation knowing only  $\dot{\phi}^\alpha$ ,  $H$  and  $V_\alpha$  from the background, provided we are prepared to tolerate the nonlocal terms. In contrast with (2.33b) it is not necessary to know the second derivative  $V_{\alpha\beta}$  and we do not need a term quadratic in the derivatives  $\delta \dot{\phi}^\alpha$ . When used to obtain correlation functions of  $\zeta$  this last property reduces the number of  $n$ -point functions of the fields and their derivatives which must be computed.

With the guarantee provided by (2.33a)–(2.33b) that it is *possible* to write a purely local formula for  $\zeta$ , the nonlocal terms in (2.34b) are harmless. For computations of  $n$ -point functions, which naturally take place in Fourier space, they merely become constant factors of  $k$ . Our numerical experiments suggest that eqs. (2.34a)–(2.34b) may even be preferable

to (2.33a)–(2.33b) because there are fewer cancellations between large contributions. This is especially noticeable in models where  $\zeta$  is conserved at or after the end of inflation. Conservation relies on a delicate interplay between separate terms in  $\zeta$  which may themselves be varying quite rapidly.

### 3 Comparison with the separate universe picture

The flat-gauge results for  $\vartheta$  quoted in eqs. (2.22a)–(2.22b) show that — up to second order in fluctuations, and in coordinates where the spatial metric is diagonal — the shift vector  $N^j$  approaches zero on superhorizon scales [9, 10, 23]. In these coordinates the only surviving perturbation to the metric on superhorizon scales is the lapse  $\alpha$  which can be absorbed into a shift of time.

After making this shift the metric is unperturbed. Therefore the equations for each matter species must be those of the homogeneous, unperturbed universe, up to corrections of order  $(k/aH)^2$ , except with initial conditions displaced by the time shift necessary to remove  $\alpha$ . When promoted to all orders in fluctuations this argument constitutes the separate universe approach [7, 8, 18, 19, 24, 25]. The necessary decay of the shift vector  $N^j$  on superhorizon scales to all orders in perturbation theory was shown by Weinberg [9, 10] and later strengthened by Sugiyama, Futamase & Komatsu [23]. The conclusion is that superhorizon-sized regions evolve individually like an unperturbed universe.

This formalism can be used to study the behaviour of superhorizon-scale perturbations by comparing the behaviour of each quantity of interest on fixed spatial hypersurfaces drawn from our choice of slicing. To do so we must know how the background solutions, parametrized in terms of this slicing, change under a shift of their initial conditions [4]. Therefore, in the separate universe approach, choice of gauge is encoded as the choice of time variable [20].

**Gauge transformations in the separate universe approach.** In this section we use the separate universe approach to compute the gauge transformation between  $\delta\phi^\alpha$  and  $\zeta$ . Versions of this calculation have been given before. Anderson et al. collected formulae valid to third-order on superhorizon scales, invoking the slow-roll expansion [3]. A derivation of the second-order gauge transformation was given in ref. [4] using purely geometrical methods on the phase space of solutions to the background equations.

The flat slicing corresponds to hypersurfaces separated by equal amounts of expansion  $N$ , where  $N(t_1, t_2) = \ln a(t_2)/a(t_1)$  measures the growth of the scale factor between times  $t_1$  and  $t_2$ . The uniform-density slicing corresponds to hypersurfaces separated by equal intervals of  $\rho$ . In the separate universe approach, changing gauge from the flat to uniform density slicings corresponds to changing time variable from  $N$  to  $\rho$ .

Consider an initial spatially flat hypersurface on which the density can be written  $\rho(\phi^\alpha, \dot{\phi}^\alpha)$ . Define some fixed value  $\rho_*$  which is smaller than  $\rho$  everywhere on the hypersurface of interest, and write  $\Delta\rho = \rho_* - \rho$ . At each point  $p$  on the hypersurface we evolve the background equations of motion (with initial conditions taken from their values at  $p$ ) until the density reaches the constant value  $\rho_*$ , and record the expansion  $\Delta N$  which is accumulated. Because  $\rho$  varies over the slice  $\Delta N$  will vary from point to point. Its variation  $\delta(\Delta N)$  represents a modulation  $\det h \sim e^{6\delta(\Delta N)}$  of the proper volume on the final slice of fixed density, and therefore we can identify  $\zeta = \delta(\Delta N)$ .



**Uniform-density gauge curvature perturbation.** If  $\Delta\rho$  is not too large the expansion accumulated during this evolution can be written

$$\Delta N(p) = \left. \frac{dN}{d\rho} \right|_p \Delta\rho|_p + \frac{1}{2} \left. \frac{d^2 N}{d\rho^2} \right|_p (\Delta\rho|_p)^2 + \dots \quad (3.1)$$

It varies over the initial slice because each term is a function of position  $p$ . If the variation  $\delta\rho$  under changes of  $p$  is also not too large, then the variation in  $\Delta N$  under a change of initial location is

$$\zeta = \delta(\Delta N) = - \left. \frac{dN}{d\rho} \right|_p \delta\rho - \delta \left( \left. \frac{dN}{d\rho} \right|_p \right) \delta\rho + \frac{1}{2} \left. \frac{d^2 N}{d\rho^2} \right|_p \delta\rho^2 \quad (3.2)$$

Because our interest lies in the gauge transformation at a fixed time we have neglected terms which vanish in the limit  $\Delta\rho \rightarrow 0$ , which corresponds to coincidence of the initial and final slices.

To obtain explicit expressions we require the derivatives

$$\frac{dN}{d\rho} = -\frac{1}{6M_{\text{P}}^2 H^2 \epsilon}, \quad (3.3a)$$

$$\frac{d^2 N}{d\rho^2} = \frac{1}{(6M_{\text{P}}^2 H^2 \epsilon)^2} \left( 2\epsilon - \frac{\dot{\epsilon}}{H\epsilon} \right). \quad (3.3b)$$

Up to this point our expressions apply for an arbitrary matter theory. Specializing to the case of canonical scalar fields appropriate for inflation, the variation  $\delta(dN/d\rho)$  satisfies

$$\delta \left( \frac{dN}{d\rho} \right) = \delta\phi^\alpha \frac{\partial}{\partial\phi^\alpha} \frac{dN}{d\rho} + \delta\dot{\phi}^\alpha \frac{\partial}{\partial\dot{\phi}^\alpha} \frac{dN}{d\rho} + \dots \quad (3.4)$$

We also have the exact expression  $\rho = V/(1 - \epsilon/3)$ , from which the variation  $\delta\rho$  can be computed. The result is

$$\zeta_1^{\delta N} = \frac{1}{2M_{\text{P}}^2 H^2 \epsilon (3 - \epsilon)} \left( \dot{\phi}^\alpha \delta\dot{\phi}_\alpha + V_\alpha \delta\phi^\alpha \right) \quad (3.5a)$$

$$\begin{aligned} \zeta_2^{\delta N} = \frac{1}{2M_{\text{P}}^2 H^2 \epsilon (3 - \epsilon)} & \left( \frac{1}{2} \left[ V_{\alpha\beta} - \frac{V_\alpha V_\beta}{H^2 M_{\text{P}}^2 (3 - \epsilon)} \left( 1 + \frac{\dot{\epsilon}}{2H\epsilon^2} \right) \right] \delta\phi^\alpha \delta\phi^\beta \right. \\ & - \frac{\dot{\phi}_\alpha V_\beta + \dot{\phi}_\beta V_\alpha}{4H^2 M_{\text{P}}^2 \epsilon (3 - \epsilon)} \left( 3 - \epsilon + \frac{\dot{\epsilon}}{2H\epsilon} \right) \delta\phi^\alpha \delta\dot{\phi}^\beta \\ & \left. + \frac{1}{2} \left[ \delta_{\alpha\beta} - \frac{\dot{\phi}^\alpha \dot{\phi}^\beta}{M_{\text{P}}^2 H^2 \epsilon (3 - \epsilon)} \left( 6 - 3\epsilon + \frac{\dot{\epsilon}}{2H\epsilon} \right) \right] \delta\dot{\phi}^\alpha \delta\dot{\phi}^\beta \right). \end{aligned} \quad (3.5b)$$

The first-order term  $\zeta_1^{\delta N}$  agrees immediately with the local expression  $\zeta_1^{\text{local}}$  given in eq. (2.33a). Although  $\zeta_2^{\delta N}$  is superficially different to  $\zeta_2^{\text{local}}$  they can be made to agree using the first-order Hamiltonian constraint and the equation of motion for the background scalar field. This gives an explicit demonstration (assuming Einstein gravity) that the gauge transformation derived from the separate universe approach agrees with the one derived from traditional cosmological perturbation theory. In practice, if a local expression is required, the more compact form (2.33a)–(2.33b) is likely to be preferable.



## 4 Conclusions

In this paper we give a formula for the uniform-density gauge curvature perturbation written explicitly in terms of the scalar field fluctuation  $\delta\phi^\alpha$  defined on spatially-flat slices. This formula is needed to compute observable quantities from second-order perturbation theory, including the bispectrum  $\langle\zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2)\zeta(\mathbf{k}_3)\rangle$ .

Our results can be written in different ways using the Hamiltonian constraint. In particular, although the expressions obtained directly from cosmological perturbation theory involve ‘nonlocal’ terms which depend on the inverse Laplacian  $\partial^{-2}$  —and are therefore naïvely incompatible with the separate universe approach — we show that these terms can be removed using the constraints. After doing so the results of perturbation theory and the separate universe approach agree. Our final results, especially eqs. (2.34a)–(2.34b) are compact, simple and can be used directly in numerical calculations. We have tested their validity using integrations of the two- and three-point functions  $\langle\delta\phi^\alpha(\mathbf{k}_1)\delta\phi^\beta(\mathbf{k}_2)\rangle$  and  $\langle\delta\phi^\alpha(\mathbf{k}_1)\delta\phi^\beta(\mathbf{k}_2)\delta\phi^\gamma(\mathbf{k}_3)\rangle$ . Using these gauge transformations we confirm the expected behaviour of  $\langle\zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2)\rangle$  and  $\langle\zeta(\mathbf{k}_1)\zeta(\mathbf{k}_2)\zeta(\mathbf{k}_3)\rangle$ , including accurate conservation when all isocurvature modes become quenched.

**Comparison with Christopherson et al.** While this paper was in preparation, a preprint was released by Christopherson, Nalson & Malik which also gives an explicit expression for  $\zeta$  in terms of  $\delta\phi^\alpha$  up to second order [5].

To aid comparison, we briefly list the similarities and differences between our calculations. First, Christopherson et al. adopt a different definition of density. Our definition,  $T_{ab}n^an^b$ , gives  $\rho = \pi^2/2N^2 + (\partial\phi)^2/2a^2 + V$  expressed in coordinates adapted to the slicing, where  $\pi^\alpha \equiv \dot{\phi}^\alpha - N^m\partial_m\phi^\alpha$ . It corresponds to what Hwang & Noh called the normal frame [26]. Christopherson et al. define the density in what Hwang & Noh call the energy frame, giving  $\rho = \pi^2/2N^2 - (\partial\phi)^2/2a^2 + V$ , again in coordinates adapted to the slicing. When all wavenumbers correspond to superhorizon scales the spatial gradients decay and these expressions agree. Therefore, under the same circumstances, our definitions of the uniform density slicing will also agree.

Second, our definitions of the curvature perturbation are different. Christopherson et al. adopt the definition of Malik & Wands [6], in which the spatial metric is written (including all orders in perturbation theory)

$$h_{ij} = a^2 \left[ (1 - 2\psi_{\text{MW}})\delta_{ij} + \partial_j F_i + \partial_i F_j + \partial_i \partial_j E + \frac{1}{2}h_{ij} \right] dx^i dx^j. \quad (4.1)$$

where  $F_i$  is divergenceless, and  $h_{ij}$  is transverse and tracefree. Malik & Wands define the curvature perturbation to be  $\psi_{\text{MW}}$ . Our definition is  $\psi = (1/6)\ln\det(h_{ij}/a^2)$ , because it is this quantity which is known to be conserved on superhorizon scales [2, 7, 11]. The Malik-Wands definition  $\psi_{\text{MW}}$  is not equivalent to the determinant of  $h_{ij}$  unless  $E = F_i = h_{ij} = 0$ . In that case the first-order parts of  $\psi$  and  $\psi_{\text{MW}}$  agree, and the second-order parts are related by  $\psi_{\text{MW}|2} = \psi_2 + 2(\psi_1)^2$  [27].

Finally, we simplify our expressions using the Hamiltonian constraint, which Christopherson et al. refer to as the momentum equation. Christopherson et al. work only with cosmological perturbation theory, not the separate universe approach, and do not eliminate the nonlocal terms which appear in their expressions.

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